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ME469: Numerical Methods and Errors

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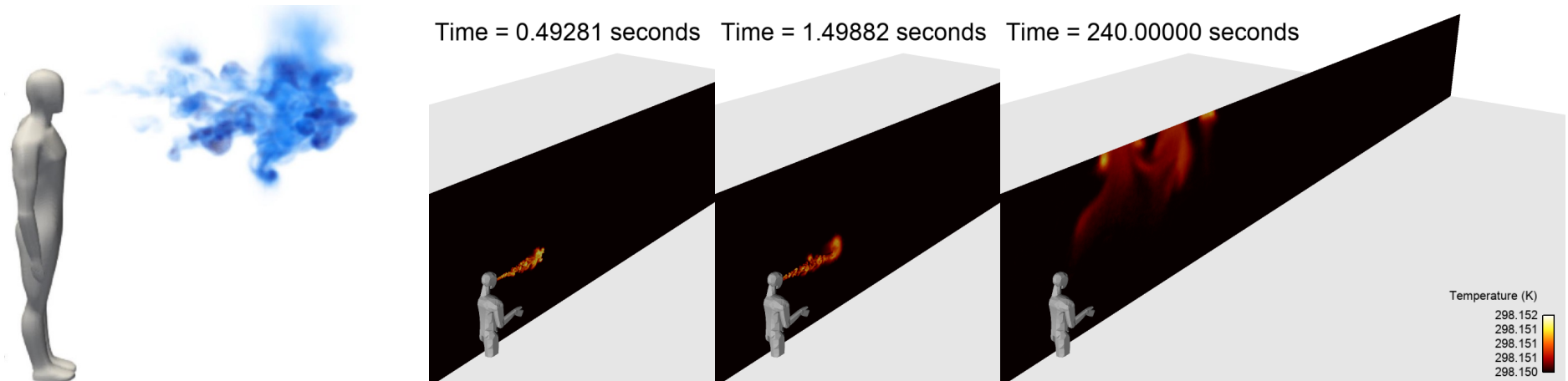
SAND2018-4536 PE





Simple Passive Scalar Transport

- The study of passive transport of nutrients or pollutants is important in biological and environmental applications (smoke, pathogens, etc.)



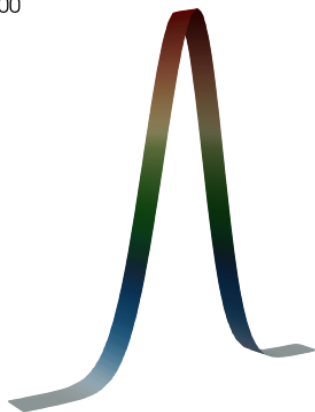
- Left, depicts a passive scalar representing a synthetic cough, Vuorinen et al. *"Modelling aerosol transport and virus exposure with numerical simulations in relation to SARS-CoV-2 transmission by inhalation indoors"*, Safety Science (2020)
- Recall that the conceptual model may require buoyancy effects, right, Domino, *"A case study on pathogen transport, deposition, evaporation and transmission: Linking high-fidelity computational fluid dynamics simulations to probability of infection"*, Int J. CFD (2021)



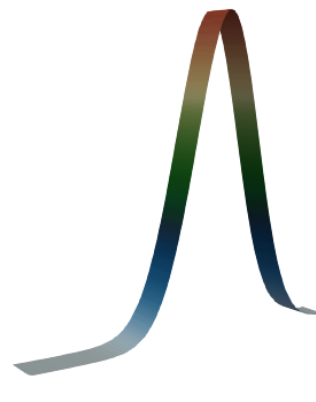
One Dimensional Temporal, Advection-Diffusion Equation Passive Scalar Transport

- Let us assume that the problem is defined in a one-dimensional configuration, and that the pollutant concentration is given by, $\phi(x,t)$
- Given an initial distribution of the pollutant $\phi(x,t = T_0)$, we can evaluate the concentration at any later time T_1 through solving a partial differential equation of the form:

Time: 0.000000



Time: 0.100000



$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2}$$

Initial Condition:

- Gaussian

Boundary Condition:

- Domain is periodic

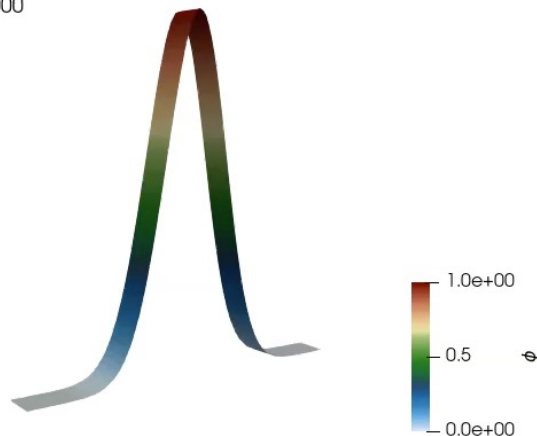
- Above, the air velocity v is constant
- Diffusion is characterized by a constant diffusivity ν , (m^2/s)



One Dimensional Temporal, Advection-Diffusion Equation Passive Scalar Transport

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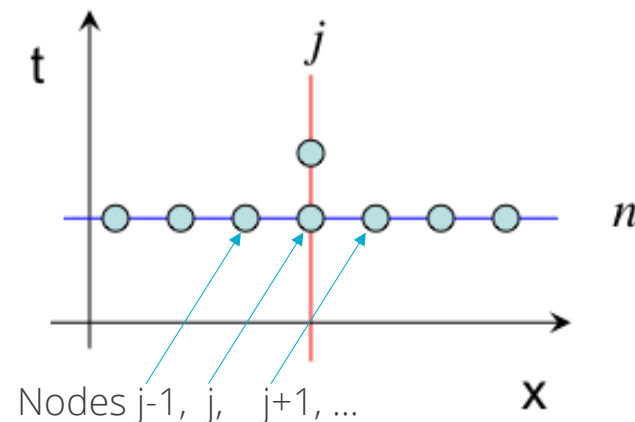
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The Discretization Step

- The region of interest ($x_L \leq x \leq x_R$) is transformed into a discrete tessellation, i.e. the grid defined by the nodes x_j or the intervals between two nodes (volume) $x_{j+1} - x_j = \Delta x$
- A similar tessellation is also used to represent time discretely in terms of level t_n or intervals $t_{n+1} - t_n = \Delta \tau$
- The solution of the original advection-diffusion equation is only sought at the specific locations (x_j) and time (t_n)

$$\phi(x_j, t^n) = \phi_j^n$$





Approximations to the Continuous Derivative

- The governing equation must also be transformed into an equivalent discrete representation
- The simplest approach involves replacing each (continuous) derivative into a discrete relationship between the function ϕ represented at the grid nodes
- Recall the formal definition of derivative:

$$\frac{\partial \phi(x)}{\partial x} = \lim_{\Delta x \rightarrow 0} \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x}$$

- Evaluated for a finite value of Δx

$$\frac{\partial \phi(x)}{\partial x} \approx \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x} \quad (+\epsilon)$$

- Note: The approximate sign represent the effect of the discretization error consequence of a non-zero Δx



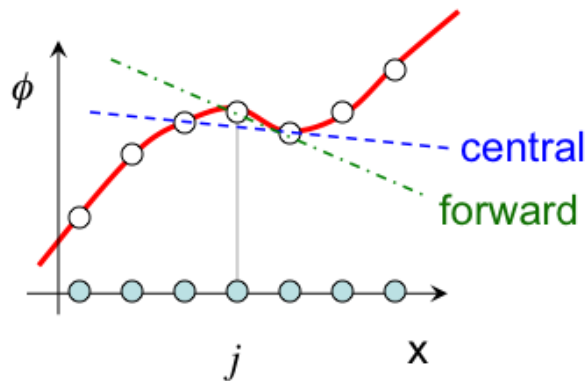
Geometric Interpretation

The formula introduced before,

$$\frac{\partial \phi(x)}{\partial x} \approx \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x}$$

is only one of the possible representations of the derivative

It can be interpreted geometrically as the approximate slope of a smooth interpolant of the discrete values ϕ_j



$$\left(\frac{\partial \phi(x)}{\partial x} \right)_j \approx \frac{\phi_{j+1} - \phi_j}{x_{j+1} - x_j}$$

forward scheme

$$\left(\frac{\partial \phi(x)}{\partial x} \right)_j \approx \frac{\phi_{j+1} - \phi_{j-1}}{x_{j+1} - x_{j-1}}$$

central scheme



Algebraic System of Equations: Explicit

- Starting from the (continuous) mathematical model:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2}$$

- The discretization step results in (discrete) computational model, for example using *forward-in-time* and *central-in-space* derivatives: FT-CS

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = \nu \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}$$

In this case the solution step is straightforward: $\phi_j^{n+1} = F(\phi_j^n, \phi_{j+1}^n, \phi_{j-1}^n, v, \nu, \Delta t, \Delta x)$

The scheme is **explicit and represents an example of a finite difference technique**: **Note: this scheme, for $\nu = 0$, is NOT STABLE (more later)**



Algebraic System of Equations: Implicit

Different choices of discretization techniques lead to more complex solution steps

- For example, *backward-in-time* and *central-in-space* derivatives: BT-CS

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} = \nu \frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2}$$

- Here, the solution step is formally: $\phi_j^{n+1} = F(\phi_j^{n+1}, \phi_{j+1}^{n+1}, \phi_{j-1}^{n+1}, v, \nu, \Delta t, \Delta x)$
- Or, better written as a Matrix system: $A\phi^{n+1} = b$

This scheme is **implicit, i.e.**, requires a matrix inversion, **and represents an example of a finite difference technique**



Many Choices on Finite Difference Operators

Derivative	Accuracy	-5	-4	-3	-2	-1	0	1	2	3	4	5
1	2					-1/2	0	1/2				
	4				1/12	-2/3	0	2/3	-1/12			
	6			-1/60	3/20	-3/4	0	3/4	-3/20	1/60		
	8		1/280	-4/105	1/5	-4/5	0	4/5	-1/5	4/105	-1/280	
2	2					1	-2	1				
	4				-1/12	4/3	-5/2	4/3	-1/12			
	6			1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90		
	8		-1/560	8/315	-1/5	8/5	-205/72	8/5	-1/5	8/315	-1/560	

Central finite difference

Derivative	Accuracy	0	1	2	3	4	5	6	7	8
1	1	-1	1							
	2	-3/2	2	-1/2						
	3	-11/6	3	-3/2	1/3					
	4	-25/12	4	-3	4/3	-1/4				
	5	-137/60	5	-5	10/3	-5/4	1/5			
	6	-49/20	6	-15/2	20/3	-15/4	6/5	-1/6		

Forward finite difference

Derivative	Accuracy	-8	-7	-6	-5	-4	-3	-2	-1	0
1	1								-1	1
	2							1/2	-2	3/2
	3						-1/3	3/2	-3	11/6

Backward finite difference

https://en.wikipedia.org/wiki/Finite_difference_coefficient



Properties of Numerical Methods

Outline:

- Consistency
- Stability, Von Neumann Analysis
- Convergence - Lax Equivalence Theorem
- Understanding Errors



High Level Concepts

A discretized mathematical model – a numerical model – is an approximation to the original, postulated, continuous model

- The properties of such numerical model have a strong effect on the computed solution

As a first step we will study three critical properties

- Consistency
- Accuracy
- Stability



Consistency

Definition: A discretization scheme for a mathematical model is consistent if it asymptotes to the original continuous form as the grid and timestep size tend to zero

- *Consistency is a property of the discretization, not of the numerical solution to the given problem*

Q: How to assess if a discretization technique is consistent?

A: Study the truncation error and verify that it vanishes as the grid and timestep size tend to zero.



Stability

Definition: A discretization scheme for a mathematical model is stable if numerical errors (e.g. round-off due to the precision in the computer representation) are not allowed to grow unbounded

- *Stability is a property of the discretization, not of the numerical solution to the given problem*

Q: How to assess if a discretization technique is stable?

A: This is fairly easy for linear PDEs with constant coefficients and no boundary conditions (periodic domains)



Stability Analysis

The simple discretization scheme (FT-CS) for the pure-advection problem is *consistent* but NOT stable

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \cancel{\nu \frac{\partial^2 \phi}{\partial x^2}}_0$$

Recall it's explicit form:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Can we understand why and, perhaps, design a different scheme that is stable?



Consistency + Stability Analysis

We can consider the effect of the truncation error as continuous terms in a modified differential equation

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Applying again a Taylor series expansion and plugging in the expression for the truncation error just found we obtain:

$$\begin{aligned} \frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} &= -\frac{\Delta t}{2} v^2 \frac{\partial^2 \phi}{\partial x^2} + O[(\Delta x)^2, (\Delta t)^2] \\ &= -\tilde{\nu} \frac{\partial^2 \phi}{\partial x^2} + O[(\Delta x)^2, (\Delta t)^2] \end{aligned}$$

- For a given Δx and Δt , note that we are not solving the pure advection equation, although the scheme is consistent (asymptotically)
- Physical viscosity (positive) has the effect of smoothing the solution; but here, the value is negative, and, therefore, **destabilizing**



Convergence

Definition: The numerical solution of a computational model approaches is convergent the exact if it asymptotes to the exact solution of the original continuous problem as the grid and timestep tend to zero

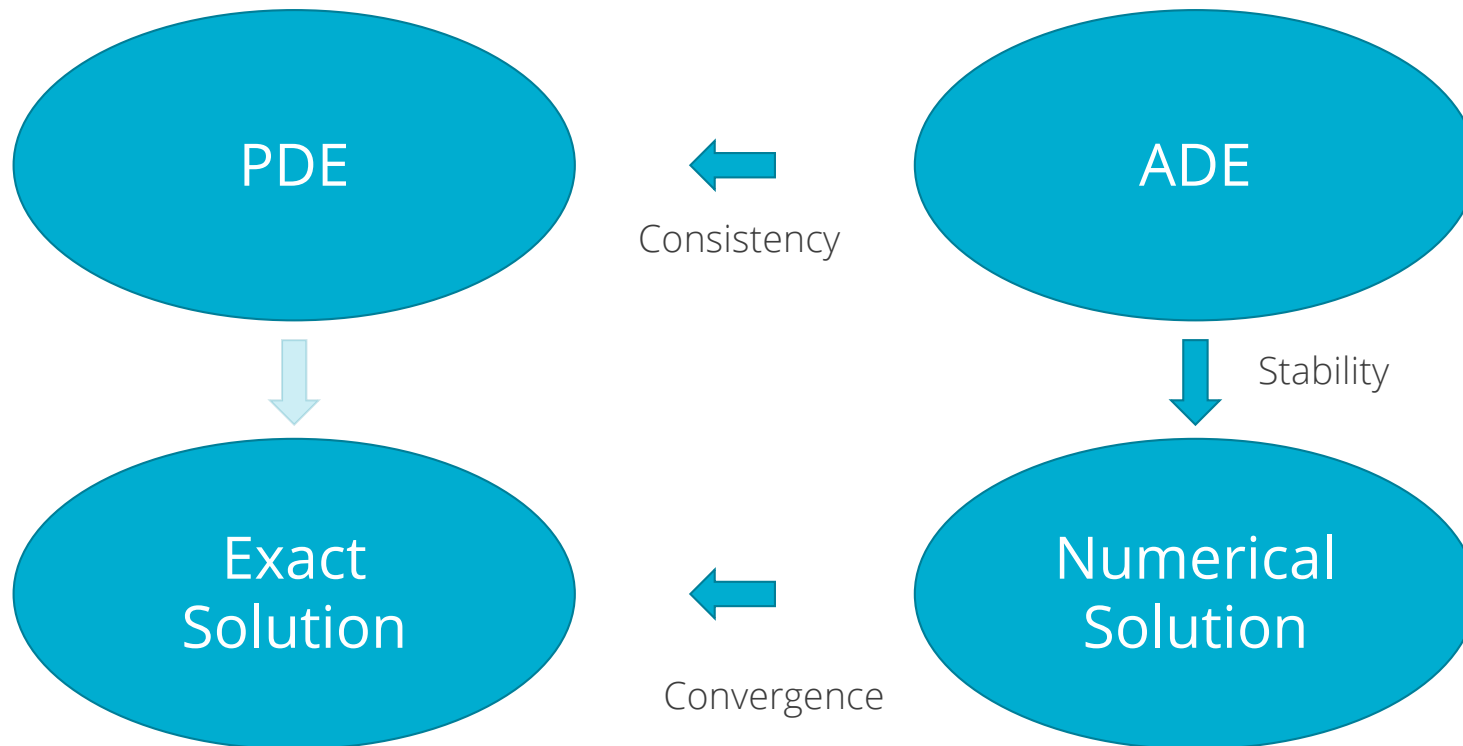
- *Convergence is a property of the solution*

Q: How to assess if the solution is converging?

A: This is formally possible only if the exact solution to the original problem is known!



Numerical Simulation Conundrum



- Convergence is required for a consistent and stable numerical method to recover the exact solution!



Lax Equivalence Theorem

Definition: For a well-posed linear problem discretized using a consistent method, stability is the necessary and sufficient condition for convergence

- In the case of a linear PDE, studying the properties of the computational method is sufficient to know that the exact solution can be computed; even before obtaining any numerical solution!
- For non-linear problems, the analysis is much harder and only weaker statements can be made
- Convergence is studied than directly and in addition to consistency and stability.



Origin of Numerical Errors

Consider again, the pure advection problem:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \cancel{\nu \frac{\partial^2 \phi}{\partial x^2}}_0$$

Recall, the *forward-in-time* and *central-in-space* scheme is consistent but unstable!

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

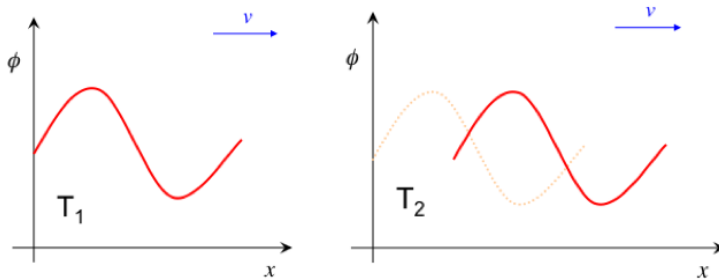
This PDE problem supports an exact solution with a simple physical interpretation

Let's use this finding to gain insight into the behavior of the numerical scheme

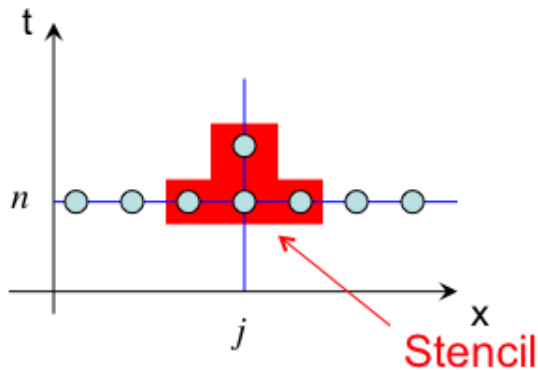


Evaluating the Exact Advection Equation Solution

Physical Interpretation: Information travels in the v -direction (positive)



Numerical Method: However, information is gathered from both $j-1$ and $j+1$ states



$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$



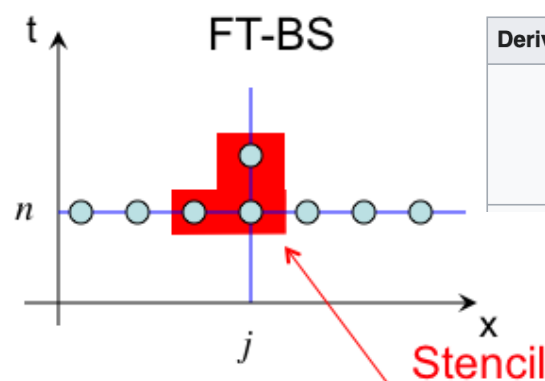
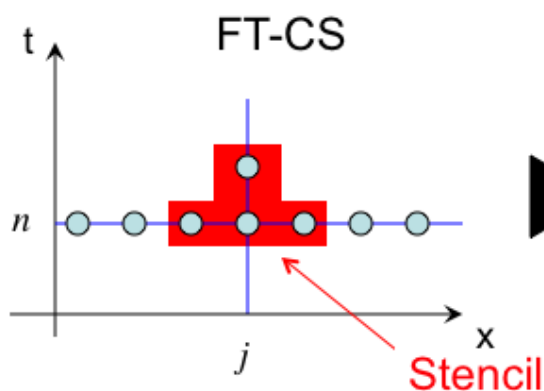
Exploiting the Directionality of the Flow

An alternative choice of spatial discretization provides a more physically-consistent discrete model: for example, if flow is moving from left to right, let's remove the $j+1$ contribution

- Consider a *forward-in-time* and *backward-in-space* differentiation (FT-BS)

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$

Recall backward finite difference stencil



Derivative	Accuracy	-8	-7	-6	-5	-4	-3	-2	-1	0
1	1								-1	1
	2							1/2	-2	3/2
	3						-1/3	3/2	-3	11/6

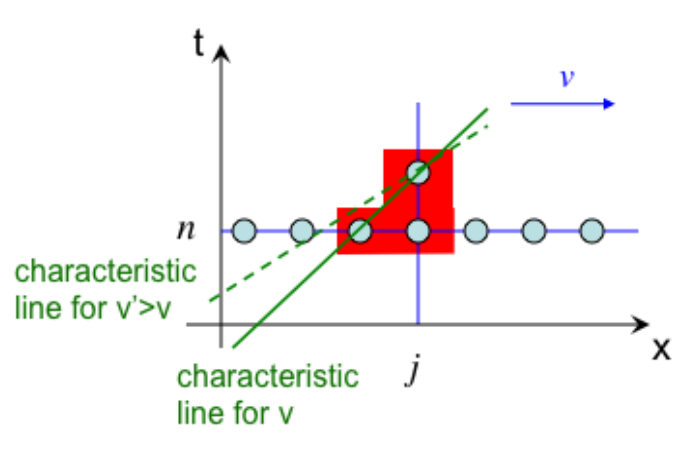
- This scheme is consistent and conditionally stable (see course reader) using Von Neumann stability analysis that shows $|\text{amplification factor}|$ is less than unity when $\frac{v\Delta t}{\Delta x} \leq 1$



Properties of the FT-BS

The scheme is consistent and conditionally stable. Why?

The characteristics lines (for fixed Δx and Δt) provide the physical picture:



Deriving the modified equation leads to a clear understanding of an underlying stabilization mechanism....



Modified Equation for the Forward-in-time, Backward-in-space

The FT-BS scheme is equivalent to:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x} (\phi_{j+1}^n - \phi_{j-1}^n) = \frac{v\Delta x}{2} \left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \right)$$

and results in the modified equation:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \frac{v\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2}$$

- The backward-in-space discretization leads to a positive dissipation, e.g. a stabilization of the scheme
- However, what happens if *velocity* < 0?



Introducing: An Upwind-based Scheme

Is it possible to simply switch between FT-BS ($v > 0$) and FT-FS ($v < 0$), while ensuring that the scheme is *consistent* and *conditionally* stable?

First, let's define an upwind and downwind operators:

$$v^+ = \frac{v + |v|}{2} \quad v^- = \frac{v - |v|}{2}$$

Furthermore, let's provide a general upwind scheme system as:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v^+ \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} + v^- \frac{\phi_{j+1}^n - \phi_j^n}{\Delta x} = 0$$

That can be reorganized as:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x} (\phi_{j+1}^n - \phi_{j-1}^n) = \frac{|v|\Delta x}{2} \left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \right)$$



Modified Equation for the Upwind-based Scheme

Recall,

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x} (\phi_{j+1}^n - \phi_{j-1}^n) = \frac{|v|\Delta x}{2} \left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} \right)$$

and results in the modified equation:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \frac{|v|\Delta x}{2} \frac{\partial^2 \phi}{\partial x^2}$$

The above form provides stabilization that is positive for all real values of velocity

Stability can also be studied using Von Nuemann analysis and results in the constraint that:

$$\frac{|v|\Delta t}{\Delta x} \leq 1$$



General Comments

- The consistency analysis and the derivation of the modified equation clearly illustrate the impact of numerical errors on the problem being solved
- The derivation of the upwind scheme shows that dissipation-like errors lead to stabilization
- What other errors can we expect to see using different discretization schemes?
- Let's re-visit the FT-CS advection system:

$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

- The truncation error for the FT-CS scheme is:

$$\epsilon = -\frac{\Delta t}{2} v^2 \left(\frac{\partial^2 \phi}{\partial x^2} \right)_j^n - v \frac{\Delta x^2}{6} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_j^n + O \left[(\Delta x)^2, (\Delta t)^2 \right]$$

- Let's examine each separately



Model 1 and Model 2 Modified Equations

Model 1:
$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$$

Model 2:
$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} + \beta \frac{\partial^3 \phi}{\partial x^3} = 0$$

Objective: Find the exact solution to these model equations in a simple periodic domain



Model 1

Postulate an expression for the solution: $\phi(x, t) = e^{pt} e^{ikx}$

Plug in the PDE: $\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$

to obtain $pe^{pt} e^{ikx} + ivke^{pt} e^{ikx} + \alpha k^2 e^{pt} e^{ikx} = 0$

This is satisfied if $p = -ivk - \alpha k^2$, leading to the solution:

$$\phi(x, t) = e^{(-ivk - \alpha k^2)t} e^{ikx} = e^{ik(x-vt)} e^{-\alpha k^2 t}$$



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$$\phi(x, t) = e^{(-ivk - \alpha k^2)t} e^{ikx} = e^{ik(x-vt)} e^{-\alpha k^2 t}$$



Model 2

Postulate an expression for the solution: $\phi(x, t) = e^{pt} e^{ikx}$

Plug in the PDE: $\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} + \beta \frac{\partial^3 \phi}{\partial x^3} = 0$

to obtain $pe^{pt} e^{ikx} + ivke^{pt} e^{ikx} - \beta ik^3 e^{pt} e^{ikx} = 0$

This is satisfied if $p = -ivk + \beta ik^3$, leading to the solution:

$$\phi(x, t) = e^{(-ivk + \beta ik^3)t} e^{ikx} = e^{ik[x - (v - \beta k^2)t]} = e^{ik(x - wt)}$$



Model 2

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Plug in the PDE: $\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} + \beta \frac{\partial^3 \phi}{\partial x^3} = 0$

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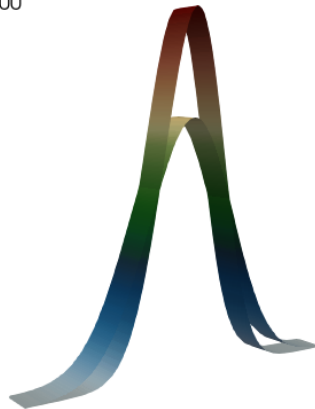
Model 1: Dissipative-like Error

Review:

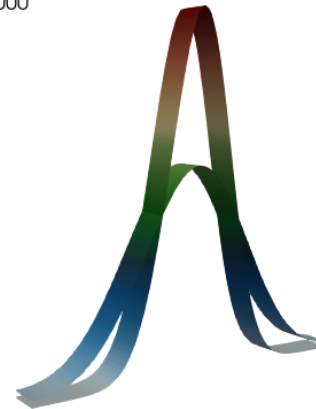
$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} - \alpha \frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\phi(x, t) = e^{(-ivk - \alpha k^2)t} e^{ikx} = e^{ik(x-vt)} e^{-\alpha k^2 t}$$

Time: 1.000000



Time: 2.000000





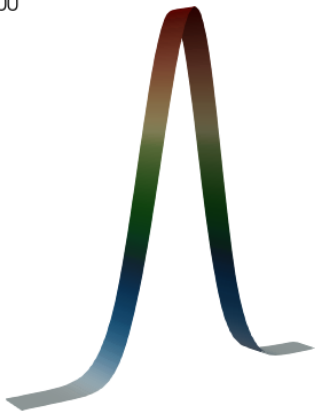
Model 2: Dispersion-like Error

Review:

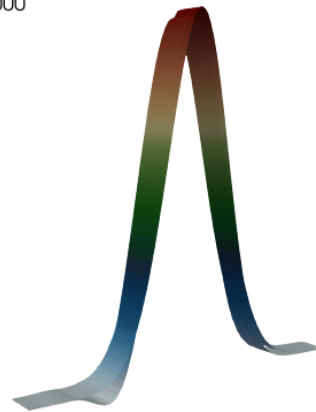
$$\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} + \beta \frac{\partial^3 \phi}{\partial x^3} = 0$$

$$\phi(x, t) = e^{(-ivk + \beta ik^3)t} e^{ikx} = e^{ik[x - (v - \beta k^2)t]} = e^{ik(x - wt)}$$

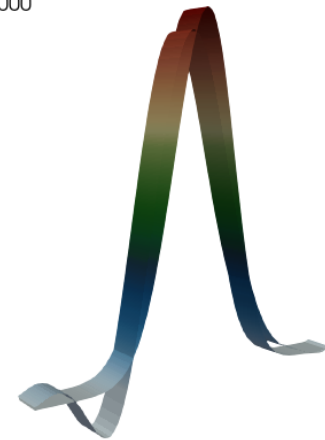
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Time: 8.000000



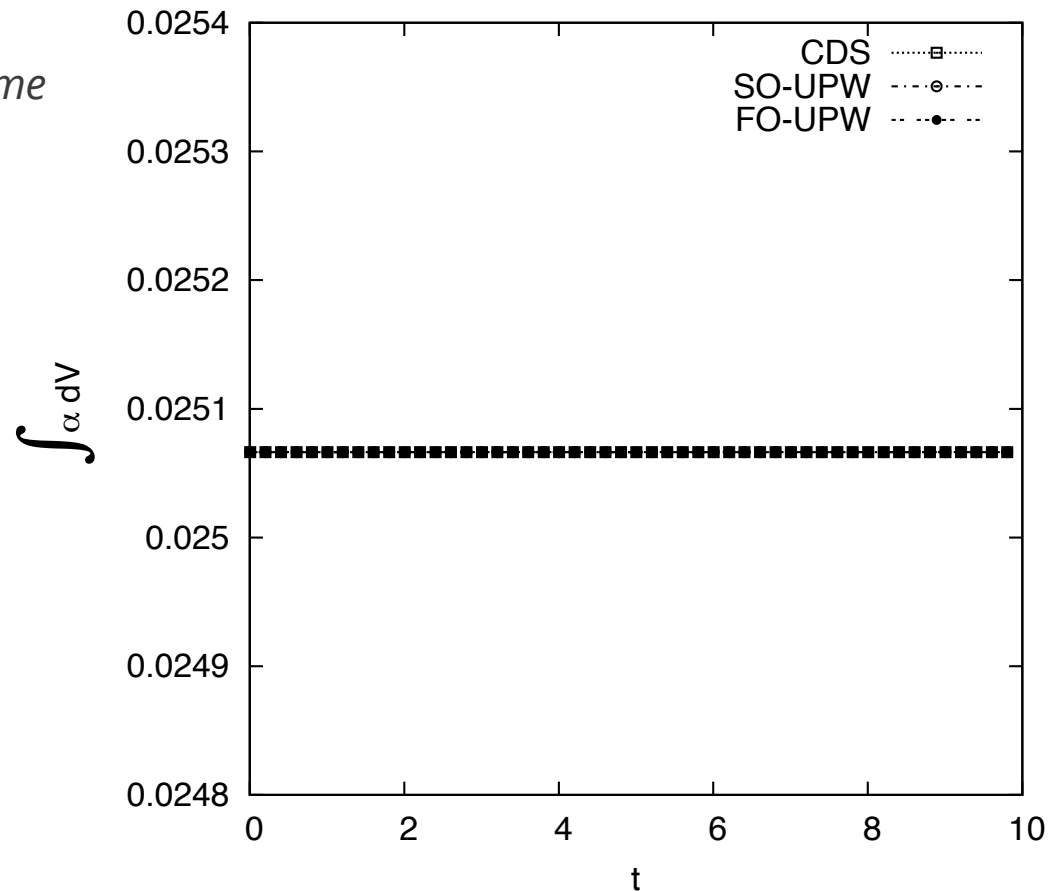


A Note on Conservation: ϕ

For our fully implicit *backward-in-time* and *central-in-space* Nalu finite volume approach:

Integration ϕ over the full domain, for any advection operator choice, results in:

- Perfect conservation





Derivation of a Energy Quantity

Starting with our model equation: $\frac{\partial \phi}{\partial t} + v \frac{\partial \phi}{\partial x} = \cancel{\nu \frac{\partial^2 \phi}{\partial x^2}}$ \downarrow
0

And scale by ϕ : $\phi \left(\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} \right) = 0$

Results in the modified equation, $\frac{\partial \frac{\phi^2}{2}}{\partial t} + u_j \frac{\partial \frac{\phi^2}{2}}{\partial x_j} = 0 \longrightarrow \frac{\phi^2}{2}$

that mimics an energy, $\frac{u_i u_i}{2}$

Let's see how this quantity is conserved....

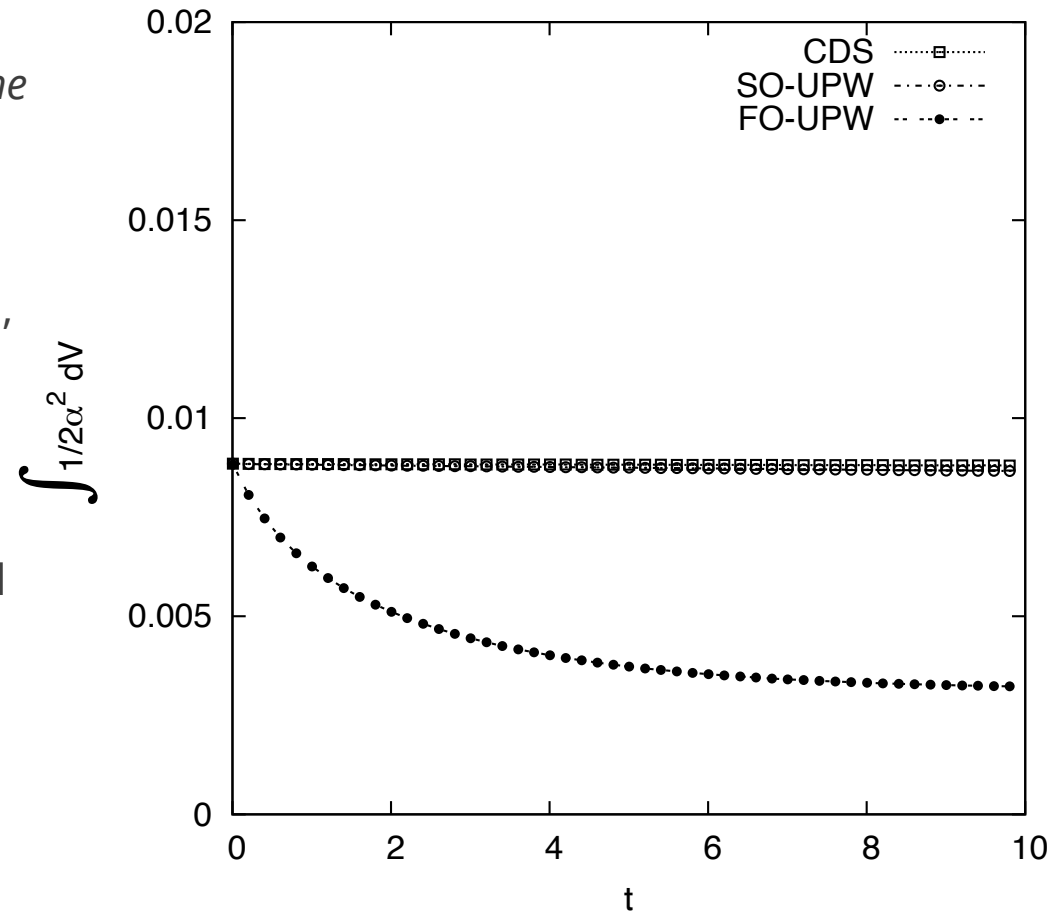


A Note on Conservation: $\phi^2/2$

For our fully implicit *backward-in-time* and *central-in-space* Nalu finite volume approach:

Integration $\phi^2/2$ over the full domain, for any advection operator choice, results in:

- Lack of conservation for the upwinded approaches
- Ideal conservation for the central operator
- Energy-method where the PDE is derived for the energy-variable, see course reader





Final Notes

- Studying the numerical properties of the discretization technique is critical to set the proper expectations on the solutions
- Classical tools such as Von Neumann stability analysis are easy to use but not generalizable
- Other properties (beyond consistency, stability, etc.) can be critical.
 - We will introduce *conservation*, *boundedness* and *symmetry*.
- Good understanding of the physics of the problem leads to better choices for the numerical schemes